

# Scalable reconstruction of density matrices

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Recent contributions in the field of quantum state tomography have shown that, despite the exponential growth of Hilbert space with the number of subsystems, tomography may still be performed efficiently by tailored reconstruction schemes. Here, we discuss a scalable method to reconstruct mixed states that are well approximated by matrix product operators. The reconstruction scheme only requires local information about the state, giving rise to a reconstruction technique that is scalable in the system size. It is based on a constructive proof that generic matrix operators are fully determined by their local reductions.

The complexity of many-body systems is one of the most intriguing, but at the same time daunting, features of quantum mechanics. The “curse of dimensionality”, namely the exponential growth of the descriptive complexity of even pure states, is a property of quantum mechanics which clearly distinguishes it from classical physics. Therefore, in general, the number of variables required to uniquely determine a quantum state increases in accordance with the growth of the Hilbert space exponentially.

Quantum state tomography addresses the problem of completely characterizing a state of a physical system by measuring a complete set of observables that determine the state uniquely [1]. As the complexity of quantum operations implemented in a laboratory steadily increases [2–4], the demand for a reliable and scalable tomography [5, 6] of prepared states is high and of considerable importance for the future of quantum technologies. The ability to store and manipulate interacting quantum many-body systems, such as linearly arranged ions in an ion trap, enhanced rapidly during the last years such that large number of quantum systems will soon be controllable for a number of particles where the conventional methods of full quantum state tomography fail due to both, the limited time that is realistically available for the experiment and the limitations to the resources that are available for the classical post-processing of the experimental data [2].

The experimental time requirement is defined by the amount of measurements which have to be done to reconstruct the state faithfully, i.e. one has to consider the system size and the number of repetitions to obtain sufficient statistics [7]. The latter is restricted by the individual tomography scheme and in particular by the representation of the state. Clearly, full quantum state tomography where the state is represented by an exponentially large number of variables will require an exponentially increasing computational power and is hence infeasible already for, e.g., trapped ion experiments available today [4]. But naturally occurring quantum states and many states of interest for quantum information tasks are completely

characterized by a number of variables scaling moderately in the number of particles: Ground states of gapped local Hamiltonians [8–10], thermal states of local Hamiltonians [10, 11], the  $W$  state, the GHZ state, and cluster states are all matrix product operators (matrix product states if they are pure) of low dimension, or very well approximated by them. These states are parameterised by a linear number of matrices of low bond-dimension. The key insight here is not that these states are matrix product operators or states (*any* state is a matrix product operator, respectively state) but that the matrix dimension is low, in particular independent of the system size. This solves one issue concerning the post-processing side of the problem mentioned above as these states may be stored efficiently on a classical computer. On the other hand, as we will see, generic matrix product operators are not only completely determined by a linear number of local observables but may also be efficiently reconstructed from such local measurements, which makes the formalism we present here a powerful tool for quantum state tomography.

Recently, it has been demonstrated that the reconstruction of pure quantum states for large systems is possible with the knowledge of local information only [5]. Here, we develop new theoretical results that permit the generalization of these ideas to mixed states. We consider  $N$   $d$ -level subsystems aligned in a one-dimensional geometry, e.g., a chain of qubits ( $d = 2$ ). The aim is to reconstruct a mixed state  $\hat{\rho}$  from local information only. The local information we have in mind are estimates to all reductions of the state to a fixed number  $R$  of contiguous sites. These may be obtained by estimating the expectation values of an informationally complete set of observables on the  $R$  sites. Note that we do not require the estimates to the reductions to be states, i.e., empirical estimates to the expectation values of local observables suffice and post-processing such as maximum likelihood estimation is not required. As  $R$  is fixed, this corresponds to an experimental effort that is linear in the system size  $N$ . We present a computationally cheap

tomography scheme, that is scaling polynomially in the system size  $N$ , which succeeds provably under a certain technical *invertibility condition* on  $\hat{\rho}$  and demonstrate numerically that it still works well when this condition is not met.

### THE SCHEME

We begin our exposition of the tomography scheme by introducing some notation. We denote the to-be-reconstructed state by  $\hat{\rho}$ . The input to the reconstruction scheme are estimates of expectation values which completely specify all reductions of  $\hat{\rho}$  to  $R$  contiguous sites. We denote these reductions by  $\hat{\rho}_k$ ,  $k = 1, \dots, N - R + 1$ . Put mathematically,  $\hat{\rho}_k = \text{tr}_{\{1, \dots, k-1\} \cup \{k+R, \dots, N\}}[\hat{\rho}]$ , i.e., the trace over all but the  $R$  sites  $\{k, \dots, k+R-1\}$ . Now let  $\{\hat{P}_i^{(\alpha)}\}_{\alpha=1, \dots, d^2}$  be a complete operator basis for the site  $i$ . A common choice for spin-1/2 particles is given by  $\hat{P}_i^{(1)} = \mathbb{1}_i/\sqrt{2}$ ,  $\hat{P}_i^{(2)} = \hat{\sigma}_i^x/\sqrt{2}$ ,  $\hat{P}_i^{(3)} = \hat{\sigma}_i^y/\sqrt{2}$ ,  $\hat{P}_i^{(z)} = \hat{\sigma}_i^z/\sqrt{2}$ , i.e., the orthonormal Pauli spin basis. We may then write

$$\hat{\rho}_k = \sum_{\alpha_1, \dots, \alpha_R} \langle \hat{P}_k^{(\alpha_1)} \dots \hat{P}_{k+R-1}^{(\alpha_R)} \rangle_{\hat{\rho}} \hat{P}_k^{(\alpha_1)} \dots \hat{P}_{k+R-1}^{(\alpha_R)}, \quad (1)$$

i.e., the  $\hat{\rho}_k$  are completely specified by the local expectation values  $\langle \hat{P}_k^{(\alpha_1)} \dots \hat{P}_{k+R-1}^{(\alpha_R)} \rangle_{\hat{\rho}} = \text{tr}[\hat{\rho} \hat{P}_k^{(\alpha_1)} \dots \hat{P}_{k+R-1}^{(\alpha_R)}]$ , estimates to which are the input to our tomography scheme.

The  $\hat{\rho}_k$  completely specify the state  $\hat{\rho}$  if a certain technical *invertibility condition* is met. The proof is constructive and gives an explicit method for obtaining  $\hat{\rho}$  from the  $\hat{\rho}_k$ . It is partly inspired by the characterization of *finitely correlated states* (as opposed to  $C^*$ -finitely correlated states) on infinite spin chains as described in the early literature [12, Prop. 2.1]. In addition to the fact that we are working in a finite and non-translation invariant setting, the main novel technical point here is that we only use *local* information, provided by the  $\hat{\rho}_k$ . To state the invertibility condition, we first need to establish some notation. We collect the  $N$  sites of the system in the set  $\mathcal{N} = \{1, \dots, N\}$ . For  $\mathcal{I} \subset \mathcal{N}$ , we define the complex vector spaces  $V_{\mathcal{I}}$  spanned by

$$\left\{ \prod_{i \in \mathcal{I}} \hat{P}_i^{(\alpha_i)} \right\}_{\alpha_i=1, \dots, d^2}. \quad (2)$$

For given  $\hat{O} \in V_{\mathcal{N}}$  and  $\mathcal{I}, \mathcal{J} \subset \mathcal{N}$  we define the linear map  $E_{\mathcal{I}}^{\mathcal{J}} : V_{\mathcal{J}} \rightarrow V_{\mathcal{N} \setminus \mathcal{I}}$  as

$$\hat{X} \mapsto E_{\mathcal{I}}^{\mathcal{J}}(\hat{X}) = \text{tr}_{\mathcal{N} \setminus \mathcal{I}}[\hat{X} \hat{O}]. \quad (3)$$

We note that the map  $E_{\mathcal{I}}^{\mathcal{J}}$  depends only on the reduction  $\hat{O}_{\mathcal{I} \cup \mathcal{J}} = \text{tr}_{\mathcal{N} \setminus \mathcal{I} \cup \mathcal{J}}[\hat{O}]$  of  $\hat{O}$  to sites  $\mathcal{I} \cup \mathcal{J}$  as

$$E_{\mathcal{I}}^{\mathcal{J}}(\hat{X}) = \text{tr}_{\mathcal{J}}[\hat{X} \hat{O}_{\mathcal{I} \cup \mathcal{J}}], \quad (4)$$

this is illustrated in Fig. 1. Note that from now on we will only consider cases where  $\mathcal{I} \cup \mathcal{J}$  is connected.

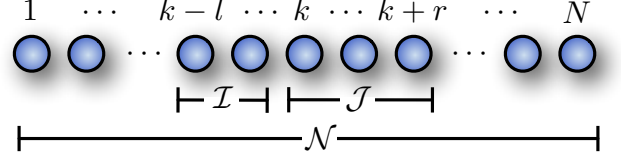


FIG. 1. Definition of the sets  $\mathcal{N} = \{1, \dots, N\}$  and  $\mathcal{I}, \mathcal{J} \subset \mathcal{N}$ . The linear map  $E_{\mathcal{I}}^{\mathcal{J}}(\hat{X}) = \text{tr}_{\mathcal{J}}[\hat{X} \hat{O}_{\mathcal{I} \cup \mathcal{J}}]$  maps operators  $\hat{X}$  (e.g. observables) living on set  $\mathcal{J}$  into operators on set  $\mathcal{I}$  by means of the reductions of  $\hat{O}$  (e.g. the state) to  $\mathcal{I} \cup \mathcal{J}$ .

**Definition 1 (Invertibility)** Let  $l, r \in \mathbb{N}$ ,  $2 \leq l+r \leq N-2$ . If  $\hat{O}$  is such that for all  $k \in \mathbb{N}$ ,  $l \leq k \leq N-r-1$ , the equality

$$\text{rank}[E_{\{k-l+1, \dots, k\}}^{\{k+1, \dots, k+r\}}] = \text{rank}[E_{\{1, \dots, k\}}^{\{k+1, \dots, N\}}] \quad (5)$$

holds, we call  $\hat{O}$   $(l, r)$ -invertible.

We may now state the main theorem, a proof of which may be found in the appendix.

**Theorem 1** Let  $l, r \in \mathbb{N}$  such that  $2 \leq l+r \leq N-2$ . Let  $\hat{O} \in V_{\mathcal{N}}$  be  $(l, r)$ -invertible. Then, for all  $\hat{X}_i \in V_{\{i\}}$ , the equality

$$\text{tr}_L[\hat{X}_1 \dots \hat{X}_N \hat{O}] = \text{tr}_L[\hat{X}_1 \dots \hat{X}_l \hat{Y}_l \hat{O}] \quad (6)$$

holds. Here, the  $\hat{Y}_l \in V_{\{l+1, \dots, l+r\}}$  are recursively defined as follows. We set  $\hat{Y}_{N-r} = \hat{X}_{N-r+1} \dots \hat{X}_N$  and

$$\hat{Y}_{k-1} = \bar{E}_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r-1\}} \left( E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{X}_k \hat{Y}_k) \right) \quad (7)$$

for  $k = l+1, \dots, N-r$ . Here, the bar indicates the Moore-Penrose pseudoinverse.

Note that, for Eq. (6) the reduction of  $\hat{O}$  to sites  $\{1, \dots, l+r\}$  is needed, for the inverse we require the reduction of  $\hat{O}$  to sites  $\{k-l, \dots, k+r-1\}$ , and for  $E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{X}_k \hat{Y}_k)$  we require the reduction of  $\hat{O}$  to sites  $\{k-l, \dots, k+r\}$ . Hence, expectation values of the form  $\text{tr}_L[\hat{X}_1 \dots \hat{X}_N \hat{O}]$  are completely specified by reductions of  $\hat{O}$  to the sites  $\{k-l, \dots, k+r\}$ ,  $k = l+1, \dots, N-r$ , i.e., by all reductions to  $R = r+l+1$  contiguous sites. By choosing the  $\hat{X}_i$  to be the basis operators  $\hat{P}_i^{\alpha_i}$ , this implies that  $(l, r)$ -invertible operators  $\hat{O}$  may be fully reconstructed from their reductions to  $R$  consecutive sites, which is the same as knowing the expectation values

$$\text{tr}[\hat{P}_k^{\alpha_k} \dots \hat{P}_{k+R-1}^{\alpha_{k+R-1}} \hat{O}], \quad \alpha_i = 1, \dots, d^2, \quad (8)$$

for all  $k = 1, \dots, N-R+1$ .

Now, of course, experimentally, the exact expectation values are only known to within a certain statistical error  $\sigma$  (commonly the estimated standard deviation of the mean after a finite number of measurements). This error propagates into the singular values of the map  $E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r-1\}}$ . As this map needs to be inverted, even small errors on singular values close to zero will lead to a large error in the reconstruction. This issue may be avoided by using *stochastic robust approximation* techniques [15], see the appendix for details.

In the appendix, we also show that a vast majority of matrix product operators fulfil the invertibility condition, i.e., a vast majority of matrix product operators may be reconstructed from local reductions alone. As noted above, practically relevant states are (well approximated by) matrix product operators of low dimension, i.e., we expect the scheme to work for a large class of mixed states. In the next section, we present numerical results for states that do not necessarily fulfil the invertibility condition and for which the local expectation values are subject to inevitable statistical noise.

## NUMERICAL EXPERIMENTS

We restrict our attention to qubits,  $d = 2$ , and illustrate the behaviour of the tomography scheme for two different classes of mixed states: (i) Thermal states of local Hamiltonians and (ii) mixed states obtained by tracing out parts of a matrix product state. We simulate the measurements in the following way. We first compute the exact local expectation values  $p_{\alpha_1, \dots, \alpha_R}^k = \langle \hat{\sigma}_k^{(\alpha_1)} \dots \hat{\sigma}_{k+R-1}^{(\alpha_R)} \rangle_{\hat{\rho}}$ ,  $\alpha_i = 0, x, y, z$ , for all  $k$ . Statistical noise is then simulated by adding random numbers (drawn from a Gaussian distribution with zero mean and standard deviation  $\sigma$ ) to them. The resulting  $\tilde{p}_{\alpha_1, \dots, \alpha_R}^k$  then serve as the input to our reconstruction scheme. At this point we would like to stress again that experimental estimates (here simulated by the  $\tilde{p}_{\alpha_1, \dots, \alpha_R}^k$ ) to the local expectation values suffice. Of course, these do not necessarily correspond to a state. We compare the reconstructed state  $\hat{\rho}_{\text{rec}}$  to the exact state  $\hat{\rho}$  by computing the Hilbert-Schmidt norm difference  $D(\hat{\rho}, \hat{\rho}_{\text{rec}}) = \|\hat{\rho}_{\text{rec}} - \hat{\rho}\|^2 / \|\hat{\rho}\|^2$ . To obtain meaningful results, we have rescaled the norm such that the deviations are measured in units of  $\|\hat{\rho}\|^2$ , the natural length scale of the state to be learned.

As a first example, we consider thermal states of the Ising Hamiltonian at its quantum critical point

$$\hat{H} = - \sum_{i=1}^{N-1} \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x - \sum_{i=1}^N \hat{\sigma}_i^z. \quad (9)$$

We obtain the thermal states by an imaginary time evolution [13, 14] using the time evolving block decimation algorithm (TEBD). From these states, we compute

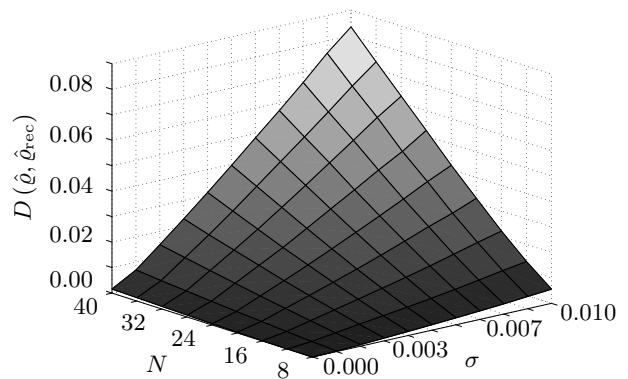


FIG. 2. Quality of our reconstruction scheme for thermal states of the Ising Hamiltonian in Eq. (9) for  $\beta = 5$  and  $R = 5$ , i.e., the state is reconstructed from local expectation values on five consecutive sites. For each pair  $(N, \sigma)$ , the plot shows the mean of the norm difference obtained from 100 realizations and renormalized by the purity of the exact state, i.e.  $D(\hat{\rho}, \hat{\rho}_{\text{rec}}) = \|\hat{\rho}_{\text{rec}} - \hat{\rho}\|^2 / \|\hat{\rho}\|^2$ . This corresponds to 100 experiments, each of which carries an uncertainty of  $\sigma$  about the local expectation values.

the exact local expectation values  $p_{\alpha_1, \dots, \alpha_R}^k$ ,  $\alpha_i = 0, x, y, z$  for all  $k$ , simulate the measurements by adding random numbers, and reconstruct the state by means of the noisy local expectation values. In Fig. 2, we show the norm difference for the exact and the reconstructed states as a function of the system size  $N$  and the error  $\sigma$ . It indicates

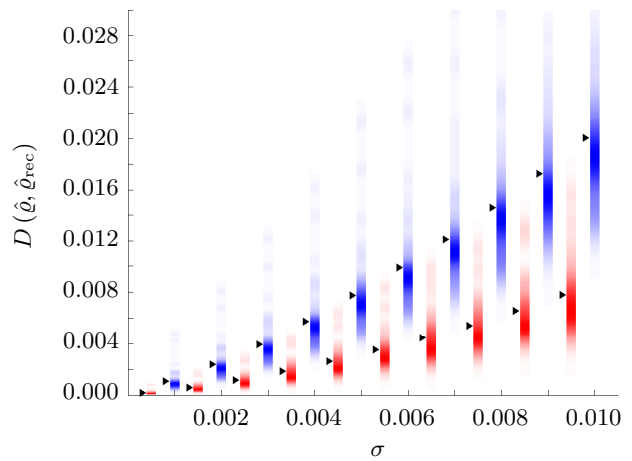


FIG. 3. Quality of our reconstruction scheme for thermal states of randomly chosen next-neighbour Hamiltonians as in Eq. (10) with  $\beta = 2$  and  $R = 5$ , i.e. the state is reconstructed from local expectation values on five consecutive sites. Red: system size  $N = 16$ , blue: system size  $N = 32$ . We generate 50 different random Hamiltonians and compute their corresponding thermal states using the TEBD algorithm. For each state and pair  $(N, \sigma)$ , the density plot shows the simulations of one experiment carrying an uncertainty of  $\sigma$  about the local expectation values. Mean values are indicated as triangles.

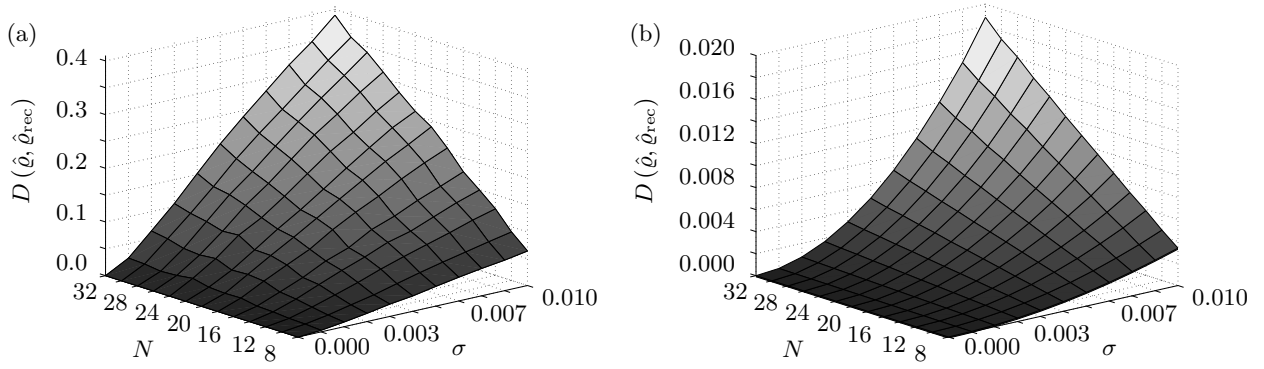


FIG. 4. Reconstruction errors for randomly chosen matrix product operators as described in the text with  $|\mathcal{N}_{\text{aux}}| = N$ . The interaction is weak in a sense that we choose  $t$  such that  $t\|\hat{H}_k\|_{\text{op}} = 1/100$  for all  $k$ . For each pair  $(N, \sigma)$  we draw 4000 random states, simulate one measurement each and reconstruct the state with the disturbed local expectation values. The plot shows the mean values of the renormalized norm differences in dependence on the system size  $N$  and the error in the measurements  $\sigma$ . (a) The states are reconstructed with  $R = 3$ , i.e. measurements are done on all blocks of three contiguous sites. Here, for given  $N$  ( $\sigma$ ), the scaling of  $D(\hat{\rho}, \hat{\rho}_{\text{rec}})$  is roughly linear in  $\sigma$  ( $N$ ). (b) Reconstruction with  $R = 5$ .  $D(\hat{\rho}, \hat{\rho}_{\text{rec}})$  improves significantly when measuring on larger blocks.

that, for given  $N$ , the error  $D(\hat{\rho}, \hat{\rho}_{\text{rec}})$  scales roughly as  $\sigma$ , similarly, for given  $\sigma$ , it scales roughly as  $N$ .

Thermal states of random next-neighbour Hamiltonians of the form

$$\hat{H} = \sum_{i=1}^{N-1} \hat{r}_{i,i+1}^i \quad (10)$$

serve as our second example. Here, the  $\hat{r}_{i,i+1}^i$  are Hermitian matrices acting on sites  $i$  and  $i+1$  with entries that have real and imaginary part picked from a Gaussian distribution with zero mean and standard deviation one. Again, we use the TEBD algorithm to obtain the exact thermal states. For each system size we generate 50 random Hamiltonians and their corresponding thermal states and simulate one experiment for each  $\sigma$  and state. Fig. 3 shows the error of the reconstructions as a function of the error of the measurements for two different system sizes. The densities illustrate the distribution of the error for the 50 different states while the black arrows indicate the mean.

Let us finally analyse the behaviour of the algorithm for states which are exactly representable as matrix product operators satisfying the invertibility condition but subject to statistical noise. We pick such matrix product operators at random by generating a matrix product state with bond-dimension  $D = d$  where the entries of the matrices defining the states are drawn from a Gaussian distribution with zero mean and standard deviation one. Then, we let these sites interact with an auxiliary system each of dimension  $d$  according to the unitary  $\hat{U}_k = e^{-i\hat{H}_k t}$  for  $k = 1, \dots, |\mathcal{N}_{\text{aux}}|$ , where  $\hat{H}_k$  is a two-particle interaction Hamiltonian acting on site  $k$  and its auxiliary system with entries picked from a Gaussian distribution with zero mean and standard deviation one. Finally, we trace

over the  $|\mathcal{N}_{\text{aux}}|$  auxiliary sites to obtain a matrix product operator with bond-dimension  $D = d^2$ . Fig. 4 shows the results for different system sizes and different noise levels and further outlines the influence of enlarging the number of measured observables. Again, the numerical results suggest that the scaling of our scheme is polynomial in both,  $N$  and  $\sigma$ .

## CONCLUSIONS

In this work we have continued the programme for efficient quantum state tomography initiated in [5] and presented a scheme to reconstruct mixed states from local measurements efficiently. We have shown that practically relevant states may be reconstructed from reductions to contiguous sets of sites alone. Further, the impact of statistical noise and the performance of the reconstruction scheme for states that do not necessarily fulfil the condition which guarantees perfect reconstruction have been investigated numerically in detail. For all simulations the Hilbert-Schmidt norm difference (normalized by the purity of the exact state) between the exact state and the reconstructed state was obtained and the numerical results suggest that the quality of the reconstruction scales algebraically in  $N$  and  $\sigma$ . The methods presented here overcome an important challenge of tomography and open the path for their application to very large systems in concrete experiments.

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  - [14] To generate the thermal states we use a fourth order Trotter expansion and adjust the step size in the imaginary time evolution to  $\delta T = 10^{-3}$  for the Ising Hamiltonian and the random next-neighbour Hamiltonians, respectively, i.e.  $\hat{\rho} = (e^{-\delta T \hat{H}})^{\beta/\delta T} / Z$ . Further, we keep the 100 largest singular values in each decomposition, i.e. ap-

proximate the state as a matrix product operator with bond-dimension  $D = 100$ .

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## APPENDIX

### Reconstructing invertible states

Here, we proof the main theorem. We start by showing that for all  $k = l + 1, \dots, N - r$ , Eq. (7) implies

$$E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r-1\}}(\hat{Y}_{k-1}) = E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{X}_k \hat{Y}_k). \quad (11)$$

To this end, we define the linear map  $\phi : \text{ran}[E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}] \rightarrow \text{ran}[E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r\}}]$ , where the domain and the range of  $\phi$  are the ranges of the denoted linear maps, as

$$\begin{aligned} \phi(E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{Z})) &= \text{tr}_{1, \dots, k-l-1} [E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{Z})] \\ &= E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{Z}), \end{aligned} \quad (12)$$

i.e.,  $\text{ran}[\phi] = \text{ran}[E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r\}}]$ , and therefore, by the rank-nullity theorem,

$$\begin{aligned} \dim[\ker[\phi]] &= \text{rank}[E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}] - \text{rank}[E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r\}}] \\ &\leq \text{rank}[E_{\{1, \dots, k-1\}}^{\{k, \dots, N\}}] - \text{rank}[E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r-1\}}] \\ &= 0 \end{aligned} \quad (13)$$

due to the invertibility condition Eq. (5). Hence,  $\phi(\hat{Z}) = 0$  is equivalent to  $\hat{Z} = 0$ , i.e., Eq. (11) is equivalent to

$$\phi(E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{Y}_{k-1} \otimes \mathbb{1})) = \phi(E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{X}_k \hat{Y}_k)), \quad (14)$$

which is implied by Eq. (7). The theorem now follows by induction over  $k = N - r - 1, \dots, l + 1$ , starting at  $k = N - r - 1$ : Eq. (5) guarantees the existence of  $\hat{Y}_{N-r-1} \in V_{\{N-r, \dots, N-1\}}$  such that

$$\begin{aligned} E_{\{1, \dots, N-r-1\}}^{\{N-r, \dots, N-1\}}(\hat{Y}_{N-r-1}) &= E_{\{1, \dots, N-r-1\}}^{\{N-r, \dots, N\}}(\hat{X}_{N-r} \hat{Y}_{N-r}) \\ &= E_{\{1, \dots, N-r-1\}}^{\{N-r, \dots, N\}}(\hat{X}_{N-r} \hat{X}_{N-r+1} \cdots \hat{X}_N), \end{aligned} \quad (15)$$

i.e., multiplying from the left by  $\hat{X}_1 \cdots \hat{X}_{N-r-1}$  and taking the trace over  $\{1, \dots, N-r-1\}$ , we find

$$\text{tr}[\hat{X}_1 \cdots \hat{X}_N \hat{O}] = \text{tr}[\hat{X}_1 \cdots \hat{X}_k \hat{Y}_k \hat{O}] \quad (16)$$

for  $k = N-r-1$ . Suppose now that this equality holds for  $l < k \leq N-r-1$  for some  $\hat{Y}_k \in V_{\{k+1, \dots, k+r\}}$ . We now show that it then also holds for  $l \leq k-1 \leq N-r-2$ . Eq. (5) guarantees the existence of  $\hat{Y}_{k-1} \in V_{\{k, \dots, k+r-1\}}$  such that

$$E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r-1\}}(\hat{Y}_{k-1}) = E_{\{1, \dots, k-1\}}^{\{k, \dots, k+r\}}(\hat{X}_k \hat{Y}_k), \quad (17)$$

multiplying from the left by  $\hat{X}_1 \cdots \hat{X}_{k-1}$  and taking the trace over  $\{1, \dots, k-1\}$ , we find

$$\begin{aligned} \text{tr}[\hat{X}_1 \cdots \hat{X}_N \hat{O}] &= \text{tr}[\hat{X}_1 \cdots \hat{X}_k \hat{Y}_k \hat{O}] \\ &= \text{tr}[\hat{X}_1 \cdots \hat{X}_{k-1} \hat{Y}_{k-1} \hat{O}], \end{aligned} \quad (18)$$

the desired equality for  $l \leq k-1 \leq N-r-2$ .

### Generic matrix product operators are invertible

Now consider matrix product operators

$$\hat{O} = \sum_{\alpha_1, \dots, \alpha_N} P_1[\alpha_1] \cdots P_N[\alpha_N] \hat{P}_1^{(\alpha_1)} \cdots \hat{P}_N^{(\alpha_N)}, \quad (19)$$

with  $P_1[\alpha] \in \mathbb{C}^{1 \times D_1}$ ,  $P_N[\alpha] \in \mathbb{C}^{D_N \times 1}$ , and  $P_i[\alpha] \in \mathbb{C}^{D_i \times D_{i+1}}$  for  $i = 2, \dots, N-1$ . We assume w.l.o.g. that  $\hat{P}_i^{(0)} \propto \mathbb{1}_i$  for all  $i = 1, \dots, N$ .

**Lemma 1** *Let  $l, r \in \mathbb{N}$  such that  $2 \leq l+r \leq N-2$ . Let  $\hat{O}$  be a matrix product operator as in Eq. (19). If  $\text{tr}[\hat{O}] \neq 0$  and for all  $k \in \mathbb{N}$ ,  $l \leq k \leq N-r-1$ , the sets*

$$\{P_{k-l+1}[\alpha_{k-l+1}] \cdots P_k[\alpha_k]\}_{\alpha_{k-l+1}, \dots, \alpha_k} \quad (20)$$

*span  $\mathbb{C}^{D_{k-l+1} \times D_{k+1}}$  over  $\mathbb{C}$  and the sets*

$$\{P_{k+1}[\alpha_{k+1}] \cdots P_{k+r}[\alpha_{k+r}]\}_{\alpha_{k+1}, \dots, \alpha_{k+r}} \quad (21)$$

*span  $\mathbb{C}^{D_{k+1} \times D_{k+r+1}}$  over  $\mathbb{C}$ , then  $\hat{O}$  is  $(l, r)$ -invertible.*

*Proof.* For  $\hat{X} \in V_{\{k+1, \dots, k+r\}}$ ,

$$\hat{X} = \sum_{\alpha_{k+1}, \dots, \alpha_{k+r}} x_{\alpha_{k+1}, \dots, \alpha_{k+r}} \hat{P}_{k+1}^{\alpha_{k+1}} \cdots \hat{P}_{k+r}^{\alpha_{k+r}}, \quad (22)$$

we find

$$\begin{aligned} &E_{\{k-l+1, \dots, k\}}^{\{k+1, \dots, k+r\}}(\hat{X}) \\ &\propto \sum_{\alpha_{k-l+1}, \dots, \alpha_k} P_1[1] \cdots P_{k-l}[1] P_{k-l+1}[\alpha_{k-l+1}] \cdots P_k[\alpha_k] \\ &\quad \times \sum_{\alpha_{k+1}, \dots, \alpha_{k+r}} x_{\alpha_{k+1}, \dots, \alpha_{k+r}} P_{k+1}[\alpha_{k+1}] \cdots P_{k+r}[\alpha_{k+r}] \\ &\quad \times P_{k+r+1}[1] \cdots P_M[1] \hat{P}_{k-l+1}^{\alpha_{k-l+1}} \cdots \hat{P}_k^{\alpha_k} \\ &=: \sum_{\alpha_{k-l+1}, \dots, \alpha_k} \mathbf{w}^\dagger P_{k-l+1}[\alpha_{k-l+1}] \cdots P_k[\alpha_k] X \mathbf{v} \\ &\quad \times \hat{P}_{k-l+1}^{\alpha_{k-l+1}} \cdots \hat{P}_k^{\alpha_k} \\ &=: \Gamma(X), \end{aligned} \quad (23)$$

where the matrix

$$\begin{aligned} X &= \sum_{\alpha_{k+1}, \dots, \alpha_{k+r}} x_{\alpha_{k+1}, \dots, \alpha_{k+r}} P_{k+1}[\alpha_{k+1}] \cdots P_{k+r}[\alpha_{k+r}] \\ &\in \mathbb{C}^{D_{k+1} \times D_{k+r+1}}, \end{aligned} \quad (24)$$

the vectors

$$\begin{aligned} \mathbf{v} &= P_{k+r+1}[1] \cdots P_M[1] \in \mathbb{C}^{D_{k+r+1} \times 1}, \\ \mathbf{w}^\dagger &= P_1[1] \cdots P_{k-l}[1] \in \mathbb{C}^{1 \times D_{k-l+1}}, \end{aligned} \quad (25)$$

and the mapping  $\Gamma : \mathbb{C}^{D_{k+1} \times D_{k+r+1}} \rightarrow V_{\{k-l+1, \dots, k\}}$ . Now,  $\Gamma(X) = 0$  is equivalent to

$$\begin{aligned} 0 &= \mathbf{w}^\dagger P_{k-l+1}[\alpha_{k-l+1}] \cdots P_k[\alpha_k] X \mathbf{v} \\ &= \text{tr}[P_{k-l+1}[\alpha_{k-l+1}] \cdots P_k[\alpha_k] X \mathbf{v} \mathbf{w}^\dagger] \end{aligned} \quad (26)$$

for all  $\alpha_{k-l+1}, \dots, \alpha_k$ . Hence, if  $\{P_{k-l+1}[\alpha_{k-l+1}] \cdots P_k[\alpha_k]\}_{\alpha_{k-l+1}, \dots, \alpha_k}$  spans  $\mathbb{C}^{D_{k-l+1} \times D_{k+1}}$  over  $\mathbb{C}$ , this is equivalent to  $X \mathbf{v} \mathbf{w}^\dagger = 0$ . Now, as  $\mathbf{w} \neq \mathbf{0}$  (implied by  $\text{tr}[\hat{O}] \neq 0$ ), this is equivalent to  $X \mathbf{v} = 0$ . Hence,

$$\ker[\Gamma] = \{X \in \mathbb{C}^{D_{k+1} \times D_{k+r+1}} \mid X \mathbf{v} = 0\}, \quad (27)$$

i.e., the rank of  $\Gamma$  is equal to

$$D_{k+1} D_{k+r+1} - \dim \{X \in \mathbb{C}^{D_{k+1} \times D_{k+r+1}} \mid X \mathbf{v} = 0\}. \quad (28)$$

Now, if  $\{P_{k+1}[\alpha_{k+1}] \cdots P_{k+r}[\alpha_{k+r}]\}_{\alpha_{k+1}, \dots, \alpha_{k+r}}$  spans  $\mathbb{C}^{D_{k+1} \times D_{k+r+1}}$  over  $\mathbb{C}$ , we have

$$\text{ran}[E_{\{k-l+1, \dots, k\}}^{\{k+1, \dots, k+r\}}] = \text{ran}[\Gamma], \quad (29)$$

i.e., the rank of  $E_{\{k-l+1, \dots, k\}}^{\{k+1, \dots, k+r\}}$  is equal to

$$D_{k+1} D_{k+r+1} - \dim \{X \in \mathbb{C}^{D_{k+1} \times D_{k+r+1}} \mid X \mathbf{v} = 0\}. \quad (30)$$

As  $\mathbf{v} \neq \mathbf{0}$  (implied by  $\text{tr}[\hat{O}] \neq 0$ ), we may set  $\mathbf{v}_1 = \mathbf{v}$  and assume that there are vectors  $\mathbf{v}_i \in \mathbb{C}^{D_{k+r+1} \times 1}$ ,  $i = 2, \dots, D_{k+r+1}$ , such that  $\{\mathbf{v}_i\}_{i=1, \dots, D_{k+r+1}}$  is an orthogonal basis for  $\mathbb{C}^{D_{k+r+1} \times 1}$ . Letting  $\{\mathbf{u}_i\}_{i=1, \dots, D_{k+1}}$  an orthogonal basis for  $\mathbb{C}^{D_{k+1} \times 1}$ , we may write

$$X = \sum_{i=1}^{D_{k+1}} \sum_{j=1}^{D_{k+r+1}} x_{i,j} \mathbf{u}_i \mathbf{v}_j^\dagger, \quad (31)$$

i.e.,  $0 = X\mathbf{v} = X\mathbf{v}_1$  is equivalent to  $0 = x_{i,1}$  for all  $i = 1, \dots, D_{k+1}$ . Hence, the rank of  $E_{\{k-l+1, \dots, k\}}^{\{k+1, \dots, k+r\}}$  is equal to

$$D_{k+1} D_{k+r+1} - D_{k+1} (D_{k+r+1} - 1) = D_{k+1}. \quad (32)$$

Finally,

$$\text{rank}[E_{\{1, \dots, k\}}^{\{k+1, \dots, N\}}] \leq D_{k+1}. \quad (33)$$

### Non-invertible inputs

The main issue arising when applying the iterative scheme to experimental data is that the local reductions are not known exactly. But of course, we may simply use their estimates (which are not necessarily states) as an input to compute the maps  $E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r-1\}}$  and  $E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r\}}$ . However, as we need to compute the inverse of the former map, already a small uncertainty will lead to a large error in the inverse. This can be dealt with the method of *stochastic robust approximation* [15], in particular with the Tikhonov regularization where a smoothing factor suppresses the effect of the smallest singular values of  $E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r-1\}}$  in its inverse. This is an often used method [16, 17]. For completeness, we outline the derivation of the smoothing factor. Let us first ease notation a bit. We write

$$\begin{aligned} \hat{P}_x &= \hat{P}_{k-l}^{(\alpha_{k-l})} \dots \hat{P}_{k-1}^{(\alpha_{k-1})}, \quad x = 1, \dots, d^{2l}, \\ \hat{Q}_x &= \hat{P}_k^{(\alpha_k)} \dots \hat{P}_{k+r-1}^{(\alpha_{k+r-1})}, \quad x = 1, \dots, d^{2r}. \end{aligned} \quad (34)$$

Suppose now that one had access to the exact local expectation values. The matrix representation,  $A$ , of  $E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r-1\}}$  would then be given by

$$\begin{aligned} A_{x,y} &= \text{tr}_{k-l, \dots, k-1} [\hat{P}_x E_{\{k-l, \dots, k-1\}}^{\{k, \dots, k+r-1\}} (\hat{Q}_y)] \\ &= \text{tr} [\hat{P}_x \hat{Q}_y \hat{O}]. \end{aligned} \quad (35)$$

Instead, we have only access to the noisy version of the entries  $\text{tr}[\hat{P}_x \hat{Q}_y \hat{O}]$ . Let us denote the resulting matrix by

$B$ . Now, assume that the errors of the local expectation values  $p_{\alpha_1, \dots, \alpha_R}^k = \langle \hat{\sigma}_k^{(\alpha_1)} \dots \hat{\sigma}_{k+R-1}^{(\alpha_R)} \rangle_{\hat{\rho}}$ ,  $\alpha_i = 0, x, y, z$ , are known for all  $k$ . Here, we simulate the error as a random variable  $X$  drawn from a Gaussian distribution with zero mean and standard deviation  $\sigma$ . The errors in the measurements propagate into errors of the matrix  $A$ . In particular, we find  $B = A + G$ , where  $G_{x,y} = X/\sqrt{d^{r+l}}$  is a random matrix with entries drawn from a Gaussian distribution with zero mean and standard deviation  $\sigma/\sqrt{d^{r+l}}$ .

Now, when applying the iterative scheme we have to solve linear equations of the form  $B\mathbf{x} = \mathbf{e}$  where  $B$  is as described above and  $\mathbf{e}$  is known. Instead of directly inverting this equation, we take possible variations in the matrix  $B$  into account, implying that the entries of  $B$  are themselves prone to noise and attempting to undo the imperfect measurements. This is done by solving the statistical least-squares problem [15]

$$\min \mathbb{E} [\|(B + G')\mathbf{x} - \mathbf{e}\|^2] \quad (36)$$

where  $\mathbb{E}$  denotes the expectation value and  $G'$  is a matrix with entries that are independent random numbers drawn from a Gaussian distribution with zero mean and standard deviation  $\sigma/\sqrt{d^{r+l}}$ , just like the assumed error in the measurements. This minimization problem can be rewritten as [15]

$$\min [\|B\mathbf{x} - \mathbf{e}\|^2 + \|V\mathbf{x}\|^2] \quad (37)$$

with  $V = \sqrt{\mathbb{E}[(G')^T G']}$ . Since we assume that the entries of  $G'$  are independent random numbers with zero mean and standard deviation  $\sigma$ , we have  $\mathbb{E}[(G')^T G]_{x,y} = \delta_{x,y} \sigma^2$  such that the minimization problem reads

$$\min [\|B\mathbf{x} - \mathbf{e}\|^2 + \sigma^2 \|\mathbf{x}\|^2]. \quad (38)$$

Problems of this form are known as Tikhonov regularizations which can be solved analytically [15]. The solution is given by

$$\mathbf{x} = (B^T B + \sigma^2)^{-1} B^T \mathbf{e}. \quad (39)$$

Finally, let us denote the singular values of  $B$  by  $s_1 \geq \dots \geq s_{\min\{d^{2l}, d^{2r}\}}$  such that  $B = U S V^T$ . Then, the solution of the statistical least-square problem (36) is given by  $\bar{B} = V \bar{S} U^T$  where  $\bar{S}$  is a diagonal matrix with entries  $f_i/s_i$  where  $f_i = s_i^2/(s_i^2 + \sigma^2)$  is the desired smoothing factor.